THEORY OF ULTRASONIC BACKSCATTER FROM MULTIPHASE POLYCRYSTALLINE SOLIDS

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INTRODUCTION

Ultrasound scatters from the microscopic single crystals that constitute polycrystalline solids. The scattering originates from crystallite-crystallite variations in the density and elastic constants. For single-phase materials, each crystallite has the same density and the same crystalline symmetry. Hence, in single-phase materials scattering arises from the variation in velocity, which in turn is due to the anisotropy of the elastic constants and the more or less random orientation of the crystallites [1,2]. The situation is considerably more complicated in multiphase alloys where the density, the crystal symmetry and the elastic constants vary from crystallite to crystallite.

We analyze the phase-sensitive detection of backscattered ultrasound from multiphase polycrystalline solids in this paper. Our goal is "Given a sufficiently detailed description of the microstructure of a multiphase alloy, predict the backscattered ultrasound." Our motivation is two-fold. First, engineers attempt to control the microstructure in order to optimize mechanical properties such as strength and fracture toughness when designing alloys. A calculable theory of backscatter will, in principle, allow them consider the acoustic quietness (and its impact on inspectability) as another goal in the design process. Second, changes in the microstructure of alloys can be ascertained from backscatter measurements. This paper is part of a program aimed at developing methods of detecting hard alpha inclusions (a deleterious change in the microstructure) in titanium jet engine alloys.

An exact calculable theory of ultrasonic backscatter is not possible due to the complexity of the ultrasound/microstructure interaction. Two limiting approximations are made in order to achieve computable formulas. First, we assume that the acoustic contrast is weak; i.e. the deviations of density and velocities are small compared to the average density and velocities (the Born approximation). Basically, the analysis is restricted to that early-time portion of the backscatter signal for which acoustic attenuation is negligible [1]. The Born approximation (linear response theory) describes the ultrasonic scattering in

Review of Progress in Quantitative Nondestructive Evaluation, Vol. 12
Edited by D.O. Thompson and D.E. Chimenti, Plenum Press, New York, 1993

terms of correlation functions of the material property deviations. We emphasize that once these correlation functions are determined, the scattering problem is solved in the Born approximation [1,2].

The second limiting approximation involves the determination of the material-property correlation functions from metallographic inspection of the alloy. We assume that the alloy is, on the average, homogeneous and isotropic. We also assume that the material property deviations vary randomly and in a *statistically independent* manner from crystallite to crystallite. That is, the material property deviations of one crystallite give no information about the material property deviations of any other crystallite. The assumption of statistical independence is fairly drastic and limits the number of real world alloys that can be treated quantitatively. However, we expect that the results based on this approximation will show the qualitative features of backscattering from multiphase systems.

The basic structure of the paper is as follows. First, we introduce a model to describe the microstructure of the alloy. We then define the acoustic backscatter coefficient (the square of the figure-of-merit of Margetan et al. [3-5]). Next, the acoustic backscatter coefficient is written for multiphase media using the assumption of statistical independence. The resulting formula is then explained in terms of an intuitive model. Next, the results of the theory are compared with measurements made on a titanium jet-engine alloy. Finally, the paper is concluded with a discussion.

DESCRIPTION OF THE ALLOY'S MICROSTRUCTURE

We describe polycrystalline metals as a set of space-filling perfect single crystals that are defined by their phase, density, elastic constant and crystalline orientation. Scattering specifically due to grain boundaries and other defects is neglected. The density is described by

$$\rho(\mathbf{y}) = \sum_{\alpha}^{M} \sum_{i_\alpha}^{N_\alpha} \rho_\alpha \gamma_{i_\alpha}(\mathbf{y}) . \tag{1}$$

Here, ρ_α denotes the density a crystallite of the α-phase, while $\gamma_{i\alpha}$ denotes the characteristic function, which is defined to be one in the i_α cell and zero elsewhere. N_α denotes the number of crystallites of the α-phase, while M denotes the number of different phases. Similarly, we describe the elastic constants by

$$C_{ijkl}(\mathbf{y}) = \sum_{\alpha}^{M} \sum_{i_\alpha}^{N_\alpha} C_{ijkl,i_\alpha} \gamma_{i_\alpha}(\mathbf{y}) \tag{2}$$

Here, C_{ijkl,i_α} denotes the elastic constant of the i_α'th grain in terms of the observational reference frame; the dependence on the crystallite's orientation is implicit. We also need to define the average value of the density and elastic constants

$$\rho_o = \langle \rho(\mathbf{y}) \rangle = \sum_{\alpha}^{M} f_\alpha \rho_\alpha \,, \tag{3}$$

and

$$C^o_{ijkl} = \langle C_{ijkl}(\mathbf{y}) \rangle = \sum_{\alpha=1}^{M} f_\alpha C_{ijkl,\alpha} \,, \tag{4}$$

and

$$C_{ijkl,\alpha} = \langle C_{ijkl,\alpha}(\mathbf{y}) \rangle \,. \tag{5}$$

Here, f_α denotes the volume fraction of the α'th phase, while $C_{ijkl,\alpha}$ denotes the ensemble average of the elastic constants (effectively over the random orientations of the crystallites).

Scattering is caused by the deviation of the density and elastic constants from the average. The deviation in the density is denoted by

$$\delta\rho(\mathbf{y}) = \rho(\mathbf{y}) - \rho_o \,, \tag{6}$$

while the deviation in the elastic constants is denoted by

$$\delta C_{ijkl}(\mathbf{y}) = C_{ijkl}(\mathbf{y}) - C^o_{ijkl} \,. \tag{7}$$

We will also need the definition

$$\delta C_{ijkl,\alpha}(\mathbf{y}) = C_{ijkl}(\mathbf{y}) - C_{ijkl,\alpha} \,. \tag{8}$$

The backscattered power depends on certain correlation functions of the deviations in the material properties, e.g. $\langle \delta\rho(\mathbf{x}) \delta\rho(\mathbf{x}') \rangle$ and $\langle \delta c_{ijkl}(\mathbf{x}) \delta c_{pqrs}'(\mathbf{x}') \rangle$. For our microstructural model, the needed correlation functions are proportional to

$$\Gamma_\alpha(\mathbf{r} - \mathbf{r}') \equiv \langle \gamma_\alpha(\mathbf{r}) \gamma_\alpha(\mathbf{r}') \rangle \,. \tag{9}$$

Note that Γ_α depends on the relative coordinate, $\mathbf{x}-\mathbf{x}'$, since the material is assumed to be uniform (translationally invariant) on the macroscopic level.

ULTRASONIC BACKSCATTERING COEFFICIENT

We model the ultrasonic experiment shown in Fig.(1). A polycrystalline half-space ($z<0$) is immersed in a water bath ($z>0$). The half-space is insonified by a phase-sensitive wide-band immersion transducer that is normally oriented with respect to the surface, which ensures that the signal is primarily due to longitudinally polarized waves. We imagine that a pulse is launched from the transducer, propagates into the solid, interacts with microstructure and is reradiated back into the water, where it is measured by the same transducer. The backscattered signal, δS, is rapidly oscillating, has mean zero and appears to be nearly random. The r.m.s. value of the signal can (for early times) be described by

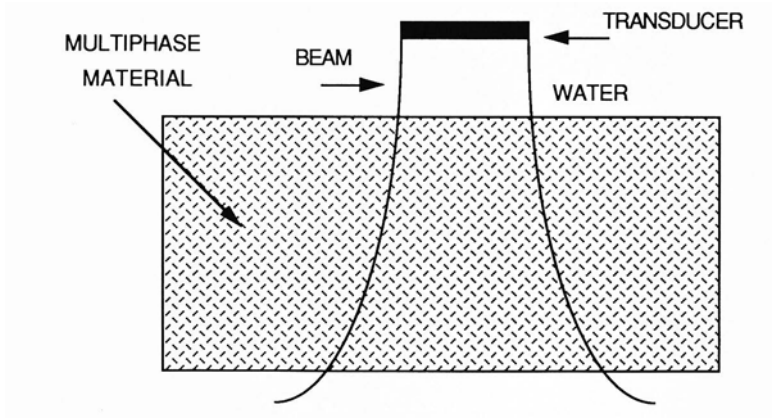

Fig. 1. Schematic representation of the backscattering experiment.

$$\left\langle |\delta S|^2 \right\rangle = \eta \int d^3\mathbf{r} |w_o(\mathbf{r})|^4 , \tag{10}$$

where, η, the acoustic backscatter coefficient, describes the power backscattered per unit volume, while w_O is a slowly varying envelope-function that describes the propagation of the beam.

We have found by detailed analysis [2] that the backscatter coefficient can be written in the intuitively simple form

$$\eta = \sum_{\alpha=1}^{M} n_\alpha \left\langle |A_\alpha|^2 \right\rangle , \tag{11}$$

for polycrystalline solids, given the two limiting assumptions mentioned above. Here, n_α denotes the number of grains per unit volume of the α'th phase. A_α denotes the (longitudinal-to-longitudinal) Born scattering amplitude for an imaginary system that consists of a single grain of the α'th phase embedded in an otherwise uniform effective medium whose density and elastic constants are determined by an average (the Voigt average) over all the grains. Equation (11) was introduced by Margetan et al. [3] on an *ad hoc* basis and has the satisfying interpretation that the total power backscattered is equal to the sum of the power backscattered from each grain independently.

The fact that the powers can be summed may be somewhat surprising, since one normally expects to sum amplitudes when considering wave scattering. The fact that one can sum the power, as well as the amplitude, arises since the deviations in the material properties of each grain are assumed statistically independent with mean zero. As a result the amplitudes of the waves scattered by each grain are statistically independent with zero mean in the Born approximation, which linearly relates the material property deviations and the scattered amplitudes. Consequently, contributions to the total scattered power that would arise due to the interference between scattering from different grain average to zero. The total power is determined by summing the power scattered by each grain.

We have evaluated the backscattering coefficient from Eqs.(9) and (10) and find

$$\eta(\omega)=\sum_{\alpha=1}^{M} f_\alpha \eta_\alpha(\omega). \tag{12}$$

Here, η_α is defined by

$$\eta_\alpha(\omega)=(R_\alpha+Q_\alpha)\mathrm{k}^4\int d^3\mathbf{u}\,\frac{\Gamma_\alpha(\mathbf{u})}{\Gamma_\alpha(0)}\exp(2ik\hat{e}\cdot\mathbf{u}). \tag{13}$$

Γ_α, the spatial correlation function defined in Eqs.(9) describes the size and distribution of the crystallites in the α'th phase. The functions R_α and Q_α describe the degree to which the material properties of the α'th phase differ (in the square) from the average. Explicitly,

$$R_\alpha(\omega)=\left(\frac{1}{(4\pi)^2}\right)\left(\frac{\delta\rho_\alpha^2}{\rho_o^2}+\frac{2\delta\rho_\alpha\langle\delta C_{11,\alpha}\rangle}{\rho_o C_{11,0}}+\frac{\langle\delta C_{11,\alpha}\rangle^2}{{C_{11,0}}^2}\right), \tag{14}$$

and

$$Q_\alpha=\frac{1}{1575\left(4\pi C_{11,0}\right)^2}\begin{pmatrix}192C_{11,\alpha}^2-128C_{11,\alpha}C_{13,\alpha}+48C_{13,\alpha}^2-256C_{11,\alpha}C_{33,\alpha}\\+32C_{13,\alpha}C_{33,\alpha}+112C_{33,\alpha}^2-256C_{11,\alpha}C_{44,\alpha}\\+192C_{13,\alpha}C_{44,\alpha}+64C_{33,\alpha}C_{44,\alpha}+192C_{44,\alpha}^2\end{pmatrix}. \tag{15}$$

Here, the single crystal elastic constants of the α'th phase are denoted by the contracted form $C_{11,\alpha}$, $C_{12,\alpha}$ etc. (note the change in notation). The expression $\langle\delta C_{11,\alpha}\rangle$ denotes the difference in the Voigt averages of C_{11} for the α'th phase and for the entire sample.

The factors R_α and Q_α in Eq.(13) have simple physical interpretations. R_α is entirely due to the multiphase nature of the sample, and is zero for single-phase materials. This part of the backscattering is due to the acoustic contrast that arises because different phases have different densities, ρ_α, and average elastic constants, $\langle C_{11,\alpha}\rangle$. It does not depend on the elastic anisotropy of the various phases. Q_α on the other hand is entirely due to the acoustic contrast that arises from the anisotropy in the elastic constants. Q_α is, in general, non zero for single-phase materials.

The frequency-dependence of the backscatter coefficient is determined if the correlation functions Γ_α are known. Preliminary experimental work indicates that Γ_α can be well described by an exponential for single-phase materials. Here we will assume that the same approximation remains reasonable for multiphase materials, i.e.

$$\Gamma_\alpha(\mathbf{r})/\Gamma_\alpha(0)=\exp(-|\mathbf{r}|/a_\alpha), \tag{16}$$

where, a_α denotes the correlation length of the α'th phase. The backscatter coefficient, evaluated using (16), is

$$\eta(\omega) = 8\pi \sum_{\alpha=1}^{M} f_\alpha (R_\alpha + Q_\alpha) \frac{k^4 a_\alpha^3}{(1+(2ka_\alpha)^2)^2} . \quad (17)$$

This is the formula that we recommend for use with multiphase polycrystalline solids. It is assumed that: (1) the material is macroscopically homogeneous and isotropic and (2) the material property deviations are statistically independent.

DEPENDENCE ON VOLUME FRACTION

In this section we analyze the dependence of the backscatter coefficient on the volume fraction for a two-phase material. The backscatter can be divided into two contributions, $\eta = \eta_R + \eta_Q$.

$$\eta_R(\omega) = 8\pi \sum_{\alpha=1}^{M} f_\alpha R_\alpha \frac{k^4 a_\alpha^3}{(1+(2ka_\alpha)^2)^2} , \quad (18)$$

and

$$\eta_Q(\omega) = 8\pi \sum_{\alpha=1}^{M} f_\alpha Q_\alpha \frac{k^4 a_\alpha^3}{(1+(2ka_\alpha)^2)^2} . \quad (19)$$

Equation (18) for η_R describes the backscattering that arises due to the contrast between the different phases. Figure (2a) shows η_R as a function of the volume fraction for a two-phase material. The density and elastic constants (Table 1) are estimates for alpha (6%Al, 1%V)and beta phase titanium (5% Al, 8% V), and were produced by using the material compositions to interpolate between elastic properties of single-crystal alpha and beta titanium. The elemental composition is appropriate for a Ti-6-4 sample produced by quenching from 900 °C. As noted above, η_R is zero for single-phase materials (i.e. when f_α is zero or one). This contribution to the backscatter is a maximum for an intermediate value of f_α. Equation (19) for η_Q describes the scattering that arises solely from the crystalline anisotropy. Figure (2b) shows the contribution, η_Q, as a nearly linear function of volume fraction for a two-phase material. This contribution would be maximized if the material were completely of the phase that has the largest crystalline anisotropy.

Table 1. Gives of the elastic constants (10^{10} dynes/cm^2) and density (g/cm^3) for the alpha (HCP) and beta (BCC) phases of Ti-6Al-4V.

PHASE	C11	C33	C12	C13	C44	ρ
ALPHA	174.4	197.3	98.1	72.0	50.7	4.54
BETA	151.2	151.2	108.0	108.0	41.1	4.48

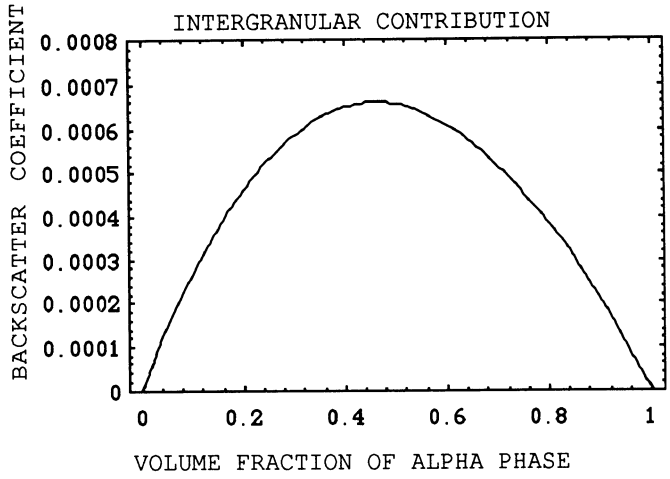

Fig. 2a. Dependence of the intergranular part of the backscattering coefficient on volume fraction.

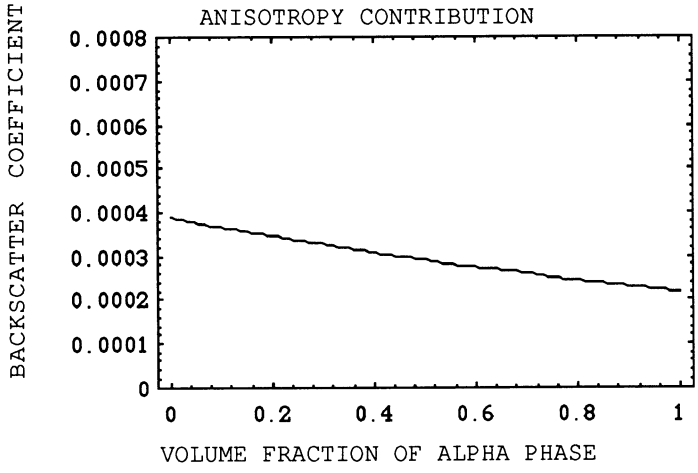

Figure 2b. Dependence of the crystalline anisotropy contribution to the backscatter coefficient on volume fraction.

APPLICATION TO AN ALPHA/BETA TITANIUM SAMPLE

Commercial alpha/beta titanium alloys are produced via a complicated process that includes forging and various heat treatments. The result is a complex microstructure that involves an acicular mixture of alpha and beta phases (see Fig. 3 of Ref. [4]). The complex needle-like microstructure has a characteristic dimension on the scale of 10 - 20 μm. There are also complex macrostructures on scales up at least several millimeters. Thompson et. al. [5] measured the backscatter coefficient for four samples of Ti-6-2-4-6. The first sample had a backscatter pattern that was nearly independent of the angle of incidence (i.e. the backscatter was nearly isotropic) and the backscatter coefficient, η, was approximately 6 10^{-4} /cm. The backscatter from three of the samples depended strongly on the

direction of incidence. The backscatter coefficient differed by a factor of roughly 100 depending on the face of the sample that was insonified (values ranged from 2.5 10^{-5} /cm to 6 10^{-3} /cm).

The analysis in this paper is almost certainly too simple to adequately model the backscatter from commercial titanium alloys. Nonetheless, it is of interest to see if the method is "in the ball park". We evaluated the backscatter from Ti-6-4 using the material properties given in Table 1. The alloy was assumed to be 50% alpha and 50 % beta phase. The correlation length was assumed to be the same for both phases and chosen so that the results of the theory agreed with the backscatter measurement from the "isotropic" Ti-6-2-4-6 sample, mentioned in the last paragraph. We found a correlation length of 12.5 μm for both phases, which is in rough agreement with the 10 - 20 μm scale of the microstructure.

SUMMARY

A calculable theory has been developed for the acoustic backscatter noise in multiphase alloy. A major simplifying assumption is that the material property deviations vary independently from grain to grain. Systematic experimental tests of the new theory are not yet available. However, the theory is consistent with the size of the backscatter noise observed in a jet engine alloy, Ti-6-2-4-6.

ACKNOWLEDGMENT

This work was sponsored by the Center for Advanced Nondestructive Evaluation, operated by the Ames Laboratory, USDOE, for the Air Force Wright Laboratory/Materials Directorate under Contract No. W-7405-ENG-82 with Iowa State University.

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